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ANNUAL REPORT ON CONTRACT N00014-89-J-3002

PRINCIPAL INVESTIGATOR: Max L Berkowitz

CONTRACT TITLE: Structure and Dynamics of Aqueous Solutions Next to and Between Membrane Surfaces.

START DATE: July 1, 1989

INTRODUCTION:

The objective of our research is to investigate structural and dynamical properties of aqueous solutions next to and between surfaces of biological macromolecules, particularly membranes. The goal of our research is to understand the molecular origin of the short-range forces acting between macromolecules. These forces are usually attributed to the polarization of water at the interface, and therefore are called hydration forces [1]. But in a recent article Israelachvili and Wennerstrom challenged this idea [2]. According to I&W, the hydration force is due to the entropic repulsion of molecular groups that are thermally excited to protrude from the surfaces. I&W claim that the monotonically repulsive hydration forces are smeared-out oscillatory forces, due to the thermal motion of the head-groups. They refer to the work of Kjellander and Marcelja [3] who performed a simulation of water between immobile lecithin molecules and obtained an oscillatory profile of water polarization. I&W claim that would the lecithin molecules be mobile the polarization profile would be monotonically decaying. Parsegian and Rand pointed out that strong discrepancies between I&W model and experiments exist[4]. It is hard to make a unique interpretation of the experiment and therefore we feel that computer simulation will play a very useful role in deciphering the nature of hydration force.

METHODS:

We use the method of molecular dynamics computer simulation in our investigation. Since phospholipid molecules are not included in a standard field force of simulation packages such as GROMOS, or AMBER or CHARMm we had to obtain potential parameters ourselves. This was done through the use of the quantum chemistry package Gaussian-88. We have also made appropriate changes in an AMBER code, that allowed us to perform molecular dynamics of a phospholipid bilayer. In addition we write our own programs to perform analysis of the data.

RESULTS AND CONCLUSIONS:

Our first simulation of water between membrane bilayers will be performed on PE/water complex. The initial configuration for the run is already prepared and is shown on figure 1. The molecular dynamics cell consist of 32 PE molecules and 242 water molecules. To find the atomic charges for the PE molecules we divided the molecule into two fragments and performed an energy optimization using Gaussian 86 at 3-26G* basis set level. Subsequently, to obtain atomic charges, the fit to electrostatic potentials was performed. At the present moment we are in a stage of preliminary molecular dynamics runs of our system.

In order to understand the general features of hydration forces we also study the structure of aqueous solutions between other macromolecules, particularly DNA molecules,

since hydration forces were also observed in this system [5]. Recently we have completed our preliminary study of structure and dynamics of water between DNA molecules [6]. We have observed that the degree of water polarization is a function of the distance between macromolecular surfaces. While the DNA molecule is trying to orient a water molecule in such a way that the dipole moment is perpendicular to the surface, the bulk water between the surfaces is trying to orient a water dipole parallel to the surface. When the surfaces are far apart the influence of bulk water between surfaces is large, and therefore the polarization of water at the surface layer is small. By bringing the surfaces closer together the influence of bulk water is diminished and the polarization of water at the interface is increased. The result is a strong increase in surface repulsion. We think that a similar polarization behavior of water may be responsible for the observed repulsive hydration forces acting between phospholipid molecules.

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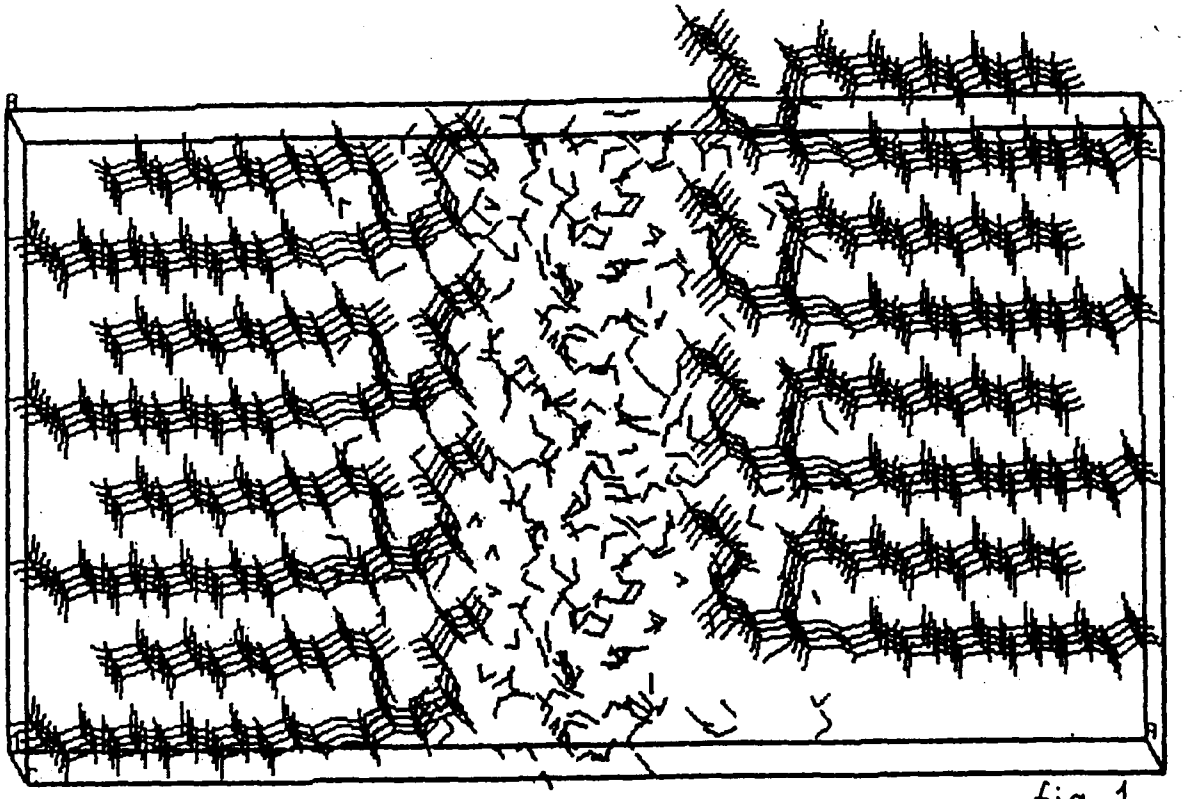

fig. 1

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